

U.S. FEDERAL INTERAGENCY WORKSHOP REVISED ANNOTATED AGENDA

"Conceptual Model Development for Subsurface Reactive Transport Modeling of Inorganic Contaminants, Radionuclides, and Nutrients"

Sponsor:

The Working Group on Subsurface Reactive Solute Transport of
Federal Interagency Steering Committee on Multimedia Environmental Models

**La Posada de Albuquerque
Albuquerque, New Mexico
April 20-22, 2004**

Description of Workshop Approach:

The proposed workshop is organized along two dimensions: applications and processes. The applications are introduced during the first day and are followed throughout the workshop. The technical review sessions are organized by processes (Physical/Coupling; Sorption; Redox/Microbiology; Precipitation/Dissolution). The breakout sessions are organized by the same topics. During the breakout sessions, we will identify research projects on the corresponding process that are directly relevant to agency applications. During the final plenary session we will pull it all together by listing the research topics that will provide the greatest benefit to the most applications.

Monday, April 19, 2004	
5:00-7:00 pm	Registration in Mezzanine and Icebreaker in Lobby (cash bar and hors d'oeuvres)
Tuesday, April 20, 2004	
7:00 am	Registration in Mezzanine and Continental Breakfast in Eulalia's Restaurant
8:00 am	Opening Session in Ball Room
8:00 am	Workshop Logistics (Malcolm Siegel - Sandia National Laboratories)
8:10 am	Welcoming Remarks (Jim Davis - U.S. Geological Survey) Description of the workshop objectives, the four technical areas to be addressed in detail, and the breakout sessions. There is a perception among the organizers of the Workshop that a "gap" exists between the conceptual models used to describe processes within the scientific research community (and at small scales) and those used in reactive transport modeling applications at the field scale. An objective of the workshop is to examine and understand the gap and make recommendations as to how it can be addressed through targeted research initiatives.
8:20 am	Plenary Session 1 - Overview of Modeling Issues in Ballroom (Session Discussion Leaders: George Yeh - University of Central Florida, Carla Koretsky - Western Michigan University)
8:20 am	Geochemistry, Groundwater and Pollution: Learning by Modeling (Tony Appelo - Hydrochemical Consultant) A review of the component parts of the governing equations, which then become the topics for individual sessions below; also a general assessment of field-scale process models in current practice and numerical implementations
8:50 am	Reactive-Transport prediction Uncertainty and Simulation Accuracy, Observation Errors, and Sensitivity Analysis (Mary Hill - U.S. Geological Survey)
9:20 am	Use of Reactive-Transport Models in Field Studies: Experience with the PHAST Simulator (David Parkhurst - U.S. Geological Survey)
9:50 am	Coffee Break in Mezzanine
10:05 am	Plenary Session 2 - Overview of Agency Applications and Modeling Needs in Ballroom (Session Discussion Leaders: Malcolm Siegel - Sandia National Laboratories, Ken Krupka - Pacific Northwest National Laboratory) Why are agencies interested in reactive transport modeling? By applications, we mean specific problems that the federal agencies are trying to solve (e.g. remediation of contaminant plumes). Brief talks describing site-specific details of representative remediation projects, risk assessments, or field studies are expected.
10:05 am	EPA Modeling Applications and Needs (Robert Puls – U.S. Environmental Protection Agency)
10:35 am	Reactive Transport Modeling of the Yucca mountain Site, Nevada (Bo Bovardsson - Department of Energy)
10:55 am	Conceptual Model Development, Remediation, and Reactive Transport Modeling at Hanford: The U.S. DOE's Largest Legacy Waste Site (John Zachara - Pacific Northwest National Laboratory)

11:15 am	NRC Modeling Applications and Needs (William Ott – Nuclear Regulatory Commission)
11:30 pm	Predicting Soil and Water Chemistry in and Below the Root Zone of Agricultural Lands: Major Ions, Nutrients and Toxic Ions (Don Suarez - Agricultural Research Service)
11:45 pm	ERDC/USACE Modeling Applications and Needs (Chris McGrath - Engineer Research and Development Center)
12:00 noon	Lunch in Eulalia's Restaurant
1:00 pm	General Discussion in Ballroom (Louise Criscenti - Sandia National Laboratories) Discussion of topics from the first two plenary sessions; further explanation of the "gap analysis" needed, reminders of the structure and goals of the workshop, and the technical and breakout sessions to come, and the workshop products that are expected.
1:20 pm	Plenary Session 3 - Physical Properties and Coupling with Reactive Processes in Ballroom (Session Discussion Leaders: Caroline Stevens – U.S. Environmental Protection Agency, Andy Tompson - Lawrence Livermore National Laboratory)
1:20 pm	Direct Visualization of Reactive Transport: Mixing at the Pore-Scale and at the Darcy-Scale (Charles Harvey - Massachusetts Institute of Technology)
1:50 pm	Modeling Fate and Transport of Inorganic-Organic Co-contaminants at a DOE Fractured Waste Site (Jack Gwo - University Maryland Baltimore County)
2:20 pm	Discussion of Plenary Session 3; discussion of scaling issues - How are the physical properties related to the conceptual model "gap" for reactive processes?
2:40 pm	Plenary Session 4 - Sorption Processes in Ballroom (Session Discussion Leaders: Bruce Honeyman - Colorado School of Mines, Janet Hering – California Institute of Technology)
2:40 pm	Radionuclide Sorption in High-Level Waste Performance Assessment: Abstraction of Results from Experiments and Surface-Complexation Models (Roberto Pabalan – Southwest Research Institute)
3:10 pm	Coffee Break in Mezzanine
3:25 pm	Plenary Session 4 - Sorption Processes in Ballroom (continued)
3:25 pm	Application of Surface Complexation Modeling to Describe Uranium(VI) Adsorption and Retardation at the Field Scale (Gary Curtis - U.S. Geological Survey)
3:55 pm	Reactive Transport Modeling of Multicomponent Ion Exchange at the Laboratory and Field Scale (Carl Steefel - Lawrence Livermore National Laboratory)
4:25 pm	Discussion of Plenary session 4; gap analysis discussion
4:50 pm	Plenary Session 5 - Discussion of the Objectives of the Breakout Sessions in Ballroom (Jim Davis - U.S. Geological Survey, John Zachara - Pacific Northwest National Laboratory) The breakout sessions will have a very focused charter, e.g. to answer the a major workshop objective: Evaluate the state of the art to define: a.) advances needed in the scientific understanding of the modeled processes, b.) new approaches for conceptual model development, c.) improved methods for assessing the values of field-relevant reaction parameters, and d.) useful targets for new model development. Attendee assignments to the breakout sessions will be made before the Workshop so that each attendee may come prepared. Technical and Breakout Session leaders and scribes will also be identified early on so that they can be prepared to ensure the smooth running and effective organization of their sessions, and delivery of Breakout Session reports. Agency representatives are encouraged to make sure that the recommendations are relevant to improving field-scale applications.
5:05 pm	Begin breakout sessions
	Working Group #1 - Physical Properties and Coupling with Reactive Processes Discussion Leaders: Carl Steefel (LLNL) and Steve Yabusaki (PNNL) Plaza Suite Working Group #2 - Sorption Processes Discussion Leaders: Louise Criscenti (SNL) and Jim Davis (USGS) Board Room Working Group #3 - Nucleation, Precipitation and Dissolution Processes Discussion Leaders: John Apps (LBNL), Alex Blum (USGS) and Ken Krupka (PNNL) Continental Room Working Group #4 - Redox Processes and Biologically Mediated Processes Discussion Leaders: Gary Curtis (USGS) and John Zachara (PNNL) Ball Room
6:00 pm	Adjourn

Wednesday, April 21, 2004	
7:00 am	Hot Breakfast Buffet in Eulalia's Restaurant
8:00 am	Opening Remarks/Logistics in Ball Room
8:10 am	Plenary Session 6 - Nucleation, Precipitation, and Dissolution Processes in Ballroom (Session Discussion Leaders: Sue Brantley - Pennsylvania State University, Janet Herman - University of Virginia)
8:10 am	Conceptual Approaches for Scaling from Molecular to Macroscopic Levels of Nucleation and Precipitation (Nita Sahai - University of Wisconsin - Madison)
8:35 am	Determining Dissolution, Precipitation and Nucleation Rate Laws in Natural Systems (Alex Blum - U.S. Geological Survey)
9:00 am	Precipitation-Front Modeling: Issues Relating to Nucleation and Metastable Precipitation in the Planned Nuclear Waste Repository at Yucca Mountain, Nevada (Eric Sonnenthal - Lawrence Berkeley National Laboratory, John Apps - Lawrence Berkeley National Laboratory)
9:30 am	Discussion of Plenary Session 6 - Gap analysis
9:55 am	Coffee Break in Mezzanine
10:10 am	Plenary Session 7 - Redox Processes and Biologically-Mediated Processes in Ballroom (Session Discussion Leaders: Dave Blowes - University of Waterloo, Tim Ginn - University of California, Davis)
10:10 am	Reactive Transport Modeling of Biologic Iron(III) Reduction Under Varied Hydrologic Conditions (Bill Burgos - Penn State University)
10:40 am	Surface Chemical and Thermodynamic Controls on Bacterial Metal Reduction in Subsurface Environments (Eric Roden - University of Alabama)
11:10 am	In-situ Biogeochemical Rate Laws in Sediments and Aquifers (Phillippe Van Capellen - Utrecht University)
11:40 am	Discussion of Plenary Session 7 - Gap analysis
12:05 pm	Lunch in Eulalia's Restaurant
1:00 pm	Plenary Session 8 - Complex Applications in Ballroom (Session Discussion Leaders: John Westall - Oregon State University, Al Valocchi - University of Illinois)
1:00 pm	Testing Coupled Microbial and Reactive Solute Transport Models with In-situ Experiments: REX and Redox Zone Experiments at Aspo (Sweden) (Javier Samper - University of La Coruna, Spain)
1:30 pm	Modeling Thermal-Hydrologic-Chemical (THC) Coupled Processes with Application to Underground Nuclear Tests at the Nevada Test Site: A "Grand Challenge" Supercomputing Problem (Peter Lichtner - Los Alamos National Laboratory)
2:00 pm	Challenges in Modeling Evolving Reactivity – Examples from Groundwater Contamination and Remediation Studies (Uli Mayer - University of British Columbia)
2:30 pm	Discussion of Plenary Session 8 - Gap analysis
2:50 pm	General Discussion: Reminder of workshop and breakout session objectives; discussion of breakout session progress from yesterday (Carl Steefel - Lawrence Livermore National Laboratory, John Apps - Lawrence Berkeley National Laboratory)
3:15 pm	Coffee Break in Mezzanine
3:30 pm	Continue breakout sessions
	Working Group #1 - Plaza Suite Working Group #2 - Board Room Working Group #3 - Continental Room Working Group #4 - Ball Room
6:00 pm	Adjourn
7:00 pm	Shuttle to Bien Shur Restaurant leaves from hotel loading zone on Copper Street

Thursday, April 22, 2004	
7:00 am	Health Nut Continental Breakfast in Mezzanine
8:00 am	Opening remarks/logistics/discussion of the breakout session progress and the products needed from the breakout sessions in Ballroom (Jim Davis - U.S. Geological Survey, Louise Criscenti - Sandia National Laboratories)
8:20 am	Continue breakout sessions
	Working Group #1 - Plaza Suite Working Group #2 - Board Room Working Group #3 - Continental Room Working Group #4 - Ball Room
10:00 am	Coffee Break in Mezzanine

10:15 am	Plenary Session 9 - Spanning the Gap: Integration of New Research and Application Ideas for Reactive Transport Modeling at the Field Scale in Ballroom (Session Discussion Leaders: Jim Davis - U.S. Geological Survey, John Zachara - Pacific Northwest National Laboratory, Carl Steefel - Lawrence Livermore National Laboratory, John Apps - Lawrence Berkeley Laboratory) This session should define how the workshop results are summarized, distributed, and used. The findings and recommendations of each breakout session, including prioritization of future research initiatives, will be presented and discussed.
12:30 pm	Closing Lunch in Eulalia's Restaurant
1:30 pm	Meetings of breakout session chairs and session scribes in Ballroom (Jim Davis - U.S. Geological Survey, John Zachara - Pacific Northwest National Laboratory, Carl Steefel - Lawrence Livermore National Laboratory, John Apps - Lawrence Berkeley Laboratory, Louise Criscenti - Sandia National Laboratories, Ken Krupka – Pacific Northwest Laboratory, Alex Blum - U.S. Geological Survey, Gary Curtis - U.S. Geological Survey, Steve Yabusaki - Pacific Northwest National Laboratory, other workshop participants welcome)
4:00 pm	Adjournment